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PERPEST MODEL, A CASE-BASED REASONING APPROACH TO PREDICT ECOLOGICAL RISKS OF PESTICIDES

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Abstract—The PERPEST model is a model that predicts the ecological risks of pesticides in freshwater ecosystems. This model simultaneously predicts the effects of a particular concentration of a pesticide on various (community) endpoints. In contrast to most effect models, PERPEST is based on empirical data extracted from the literature. This model is based on case-based reasoning, a technique that solves new problems (e.g., what is the effect of pesticide A?) by using past experience (e.g., published microcosm experiments). The database containing the past experience has been constructed by performing a review of freshwater model ecosystem studies. This review assessed the effects on various endpoints (e.g., community metabolism, phytoplankton, and macroinvertebrates) and classified them according to their magnitude and duration. The PERPEST model searches for analogous situations in the database, based on relevant (toxicity) characteristics of the compound. This allows the model to predict effects of pesticides for which no effects on a semifield scale have been published. The PERPEST model results in a prediction showing the probability of classes of effects (no, slight, or clear effects, plus an optional indication of recovery) on the various grouped endpoints. This paper discusses the scientific background of the model as well as its strengths, limitations, and possible applications.

Keywords—Effect model Aquatic community Ecological risk assessment Pesticides Case-based reasoning

INTRODUCTION

The tiered ecological risk assessment of pesticides consists of a conservative first tier and more realistic higher tiers. Suitable higher-tier studies may comprise laboratory tests that focus on more realistic exposure regimes or the testing of additional (indigenous) species, the use of computer simulation models (population, food-web, or landscape), and experiments in model ecosystems [1]. To this end, many microcosm and mesocosm experiments have been performed over the last 20 years and published in the open literature. Brock et al. [2,3] reviewed the open literature for microcosm and mesocosm experiments on the effects of herbicides and insecticides to establish ecological threshold values for pesticides in surface waters and to evaluate current standard-setting methodologies. The present paper presents a model that allows this information to be used to evaluate new cases, that is, to predict the effects of a particular concentration of a particular pesticide on aquatic ecosystems.

Effects of pesticides on aquatic communities and ecosystems can be predicted using large simulation models such as food-web models [4,5]. However, ecological models often are incomplete and usually have many uncertain parameters, making their predictions uncertain too. In fact, experts are often better able to predict effects of toxicants compared to these models. Anderson [6] has shown that past cases are used as models when trying to solve new problems. For instance, if experts are asked what the effect of 1 µg/L of the insecticide chlorpyrifos will be on the ecology of a freshwater ecosystem, they will look for analogous cases, that is, experiments they

have conducted or evaluated in the past. Obviously, the type of experimental ecosystem, test design, endpoints, and other factors will differ between the experiments, and the expert will have to take this into account. In the field of artificial intelligence, this process is called case-based reasoning (CBR) [7,8]. The principle of CBR is that it retrieves similar experience (cases) about similar situations from the memory (a database that is called the case base) and reuses this experience to make predictions in the context of a new situation.

The present paper discusses PERPEST, a model that uses case-based reasoning to predict the effects of a particular concentration of a pesticide on a defined aquatic ecosystem, based on published information about the effects of pesticides on the structure and function of aquatic ecosystems as observed in semifield experiments. The CBR system consists of the database containing this information and a search routine named weighted analogies prediction [9]. The rationale behind weighted analogies prediction is that it uses a few characteristics of the question case (e.g., exposure concentration, toxicological mode of action, and type of ecosystem) to identify analogous cases in the database. These analogous cases can then be weighted and summarized in a prediction. This means that even though no results of microcosm or mesocosm experiments have been published for a particular pesticide, it is still possible to predict its effect on a semifield scale by using the results of experiments performed with other pesticides.

The PERPEST model can be used in ecological risk assessment when uncertainties are large and data availability is poor. The PERPEST model can then provide some indication of the types of uncertainties that are likely to be large, and thus of the type of data that must be gathered for a refined risk assessment (e.g., endpoints and exposure concentrations

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Table 1. Example of two case studies, of an herbicide (atrazine) and an insecticide (chlorpyrifos)

	Atrazine	Chlorpyrifos	
Concentration (μg/L)	500	35	
References	[28-30]	[31–33]	
	Multiple/	Single/	
Exposure	constant	pulse	
	Stagnant/	Stagnant/	
Type of ecosystem	recirculating	recirculating	
Grouped endpoint (score)			
Community metabolism	3	3	
Phytoplankton	5		
Algae and macophytes		5	
Periphyton	0		
Microcrustacea		5	
Macrophytes	5		
Rotifers		1	
Zooplankton	4		
Macrocrustacea		5	
Macrocrustaceans			
and insects	4		
Insects		5	
Other macroinvertebrates	1	4	
Vertebrates	5	0	

of interest). The model can be used in both predictive (e.g., effects of a new pesticide) and retrospective (e.g., measured concentrations of a pesticide in a river) risk assessment. The PERPEST output can be used to translate spatially and temporally distributed measured or modelled concentration data into effect concentrations, that is, it can be used as a risk indicator. This paper first describes the case base that has been constructed for ecological effects of herbicides and insecticides, and then outlines the model itself and its optimization to predict particular cases. Finally, the paper discusses the model's pros and cons, together with future developments.

THE DATABASE

The database (called the case base) consist of two data sets, one containing the results of the review of the effects of pesticides observed in semifield experiments [2,3] and one containing chemical properties and ecotoxicological profiles, based on the results of standard laboratory tests of insecticides and herbicides. The first data set comprises case studies in which the effect of a particular concentration of a particular pesticide is evaluated with freshwater microcosms or mesocosms. Experiments were selected for evaluation if the model ecosystem simulated a realistic freshwater community, the experimental design was appropriate (analysis of variance or regression design), and the exposure concentrations were clearly defined. We made a distinction between systems in which a single (single or pulse) and those in which a repeated (multiple or chronic) dose was applied and between lentic (stagnant or recirculating) and lotic (flow-through) systems. The experiments evaluated normally comprised several cases, that is, each concentration evaluated in an experiment represents a separate case in the case base.

The endpoints evaluated were classified into eight different ecological endpoint groups, which were different for insecticides and herbicides (see Table 1). Within each of the eight ecological endpoint groups, the most sensitive endpoint was selected for assignment to an effect class. The responses observed for these groups were assigned to 0 or to the five effect classes, as follows. 0 = Endpoint not evaluated in the study. 1 = No effects demonstrated: no consistent adverse effects are

observed as a result of the treatment; observed differences between treated test systems and controls do not show a clear causality. 2 = Slight effects: confined responses on sensitive endpoints (e.g., partial reduction in abundance); effects observed on individual sampling dates only and/or of very short duration directly after treatment. 3 = Clear short-term effects, lasting less than eight weeks: convincing reductions on sensitive endpoints, with recovery taking place within eight weeks; effects observed on a sequence of sampling dates. 4 = Clear effects, recovery not studied: clear effects (e.g., severe reductions of sensitive taxa over a sequence of sampling dates) are demonstrated, but the monitoring of the endpoint did not last long enough to demonstrate complete recovery within eight weeks after the last treatment. 5 = Clear long-term effects, lasting more than eight weeks: convincing reductions on sensitive endpoints and complete recovery of these endpoints more than eight weeks after the last treatment; negative effects reported over a sequence of sampling dates.

A total of 90 experiments were evaluated (113 references published between 1980 and 1998). This evaluation resulted in 333 cases (substance and concentration combination), with 171 evaluating the effects of herbicides and 162 evaluating the effects of insecticides. Because eight ecological endpoint groups were evaluated, a case base of $330 \times 8 = 2,664$ entries resulted, of which 1,104 were nonzeros. Each record in the case base is composed of the name of the chemical, the concentration evaluated, the reference to the open literature, type of exposure and model ecosystem, and the effect scores for the eight ecological endpoint groups. Examples of cases are given in Table 1.

The second data set consists of laboratory fate characteristics of the different pesticides and their toxicity to standard test species. To allow comparisons between studies performed with different herbicides or insecticides, we expressed the exposure concentrations as toxic units (TU). To this end, we divided the exposure concentration studied (usually the nominal peak concentration of the pesticide in the water column) by the corresponding geometric mean acute median effect concentration (EC50) value of the most sensitive standard test species according to the Organisation for Economic Co-operation and Development (Paris, France) guidelines. In the case of insecticides, the most sensitive standard test species usually was Daphnia magna [3]. For herbicides, the most sensitive standard test algae according to the Organisation for Economic Co-operation and Development guidelines were usually Scenedesmus subspicatus or Selenastrum capricornutum [2]. By way of example, Figure 1A and B summarizes the effects of insecticides with an acetylcholinesterase toxicological mode of action on microcrustacea (Fig. 1A) and of herbicides with a photosynthesis-inhibiting toxicological mode of action on community metabolism (Fig. 1B). The figure clearly shows a concentration-effect relationship and lower effect concentrations for long-term exposure than for short-term exposure.

Analogies in terms of fate characteristics of pesticides were traced by taking into account the results of standard laboratory fate studies, such as the median dissipation time (DT50) of the water compartment determined in a water sediment study, the Henry coefficient (air—water partitioning coefficient), and the water—organic matter partitioning coefficient ($K_{\rm OM}$). When available, these variables were added to the database for each pesticide.

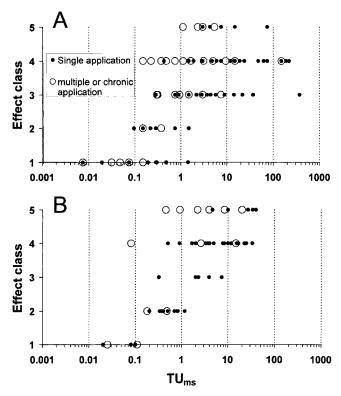


Fig. 1. Summary of effects of acetylcholinesterase-inhibiting insecticides on microcrustacea (A) and of photosynthesis-inhibiting herbicides on community metabolism (B) as observed in semifield experiments. Filled circles denote exposure regimes due to a single application; larger open circles indicate exposure due to multiple or chronic applications. The evaluated concentrations of the various pesticides are standardized on toxicity to the most sensitive standard test species (TU_{ms}). See text for description of effect class. TU = toxic unit.

CASE-BASED REASONING

Case-based reasoning is a problem-solving paradigm that is able to utilize the specific knowledge of previously experienced, concrete problem situations (cases) to solve new problems. Case-based reasoning is an approach that enables incremental, sustained learning because new experience is retained, making it immediately available for future problems [10]. Research in the early 1980s on the role of remembering earlier situations and situation patterns in problem solving and learning formed the start of CBR in artificial intelligence [11]. Kolodner [12] incorporated Schank's theory of problem solving and learning in the first CBR system that incorporated knowledge on the various travels and meetings of the former U.S. Secretary of State, Cyrus Vance. Since then, CBR studies have been driven by two primary motivations: to model human reasoning and learning and to make artificial intelligence systems more effective [8]. Case-based reasoning can be divided into two classes: interpretative CBR and problem-solving CBR. The former uses prior cases as reference points for classifying or characterizing new situations, whereas the latter uses prior cases to suggest solutions that might apply to new circumstances [7]. The present paper focuses on interpretative CBR. A very important feature of CBR is its ability to learn. Adding present experience to the case base allows improved predictions to be made in the future. Early applications of CBR include diagnostics (clinical audiology, heart failure, building defects, and aircraft fault diagnosis and repair), legal reasoning (criminal sentencing, patent law, injuries to workers, and build-

ing regulations), arbitration (dispute resolution), design (landscape, mechanical design, and conceptual design), and planning (warfare planning and manufacturing planning problems) [13]. Well-known applications of interpretative CBR in medicine include helping medical personnel to assess patient status, assisting in establishing diagnoses, and facilitating the selection of a course of therapy [14]. In this example, a case is defined as a set of variable values or features collected from a patient during a consultation or visit. This case can be compared with previously collected cases (patients) incorporated in a case base [15], from which the most similar cases can be extracted by applying, for instance, the nearest-neighbor technique. These similar cases can then be used to calculate some useful statistics such as similarities in diagnosis and successful therapy between the cases, and these statistics can be used for decision-making. Case studies play an important and useful role in medical education, and for good reason.

Case-based reasoning consists of four processes: retrieval, analogy, adaptation and learning. These are not independent processes. Retrieval of cases from the case base that are similar to the question case is driven by the definition of analogy [8]. A proper description of a CBR model should include detailed information about these processes (see next section).

THE PERPEST MODEL

This section provides definitions of the four basic CBR processes (retrieving cases, finding analogous cases, summarizing and optimizing the prediction, and learning) in PER-PEST.

Retrieving cases

Description of question case. The question case is the existing case for which risk must be estimated or the hypothetical case for which risk must be predicted. The minimum information needed to describe the question case is a chemical name, a type of pesticide, a concentration, and an EC50 for the most sensitive standard test species. The EC50 for the most sensitive test species is needed to standardize the concentration for toxicity, that is, to rescale the concentrations to TU to allow the exposure to be compared with the cases in the case base. Optional parameters, which can be used to narrow the search or weight the analogous cases, are toxicological mode of action, molecule group, DT50, K_{OM} , Henry coefficient, exposure regime, and type of ecosystem. These optional parameters enable the user to focus on chemicals with similar environmental effect and fate characteristics or ecosystems with similar structure while making the prediction.

Selection of part of the case base. Parts of the case base can be excluded from the search for analogies on the basis of characteristics of the type of chemical, exposure, and ecosystem. Thus, it is possible to exclude from the analysis all cases that differ from the question case by more than a factor of 10 TU, or all experiments performed in a lotic ecosystem.

Transformation, standardization, and weighting of variables. Before they are used to calculate similarity values between cases, it is useful to transform the different variables. The concentrations are first standardized on their toxicity to standard test species, and then log transformed by default. Other available transformations are log percentage, inverse, square root, and angular. Subsequently, all variables are standardized to mean 0 and standard deviation 1 by default to make them all equally important, that is, to remove arbitrariness in terms of measuring units. The other standardization

methods available are no standardization and MinMax standardization. In the MinMax method, the variables are scaled between the minimum and maximum values in the case base, with the minimum being allocated a value of 0 and the maximum a value of 1 [9].

After transformation and standardization, the different variables can be weighted by multiplying each with a predefined weighting factor, to give more weight to important variables. These weighting factors can be optimized by using controlled random search (see next section).

Finding analogous cases

Within the PERPEST model, one can choose between four different dissimilarity indices to calculate the distance between the question case and the retrieved cases. The default index is the Euclidean distance (ED), the others are city block distance (CB), cord distance (CD), and Chebychev distance (ChD). The ED is the index most frequently used in ecology. The ED is the distance in the *n*-dimensional space in which each variable is one dimension of the space [16]. The ED is defined as

$$ED = \sqrt{\sum_{k=1}^{n} (y_{ki} - y_{kj})^2}$$

in which y_{ki} is the transformed and standardized variable k in case i and y_{kj} is the variable k in the question case j, both multiplied by the weight of the variable k. The parameter n is the number of cases. The CB is the sum of the absolute differences between all variables [9]. The CB gives slightly lower weight to the outlying variables than the ED does and is defined as

$$CB = \sum_{k=1}^{n} |y_{ki} - y_{kj}|$$

The CD is geometrically represented by the distance between the points where the sample vectors intersect a unit sphere [16]. The CD gives more weight to qualitative aspects than the other indices. The CD is defined as

$$CD = \sqrt{\sum_{k=1}^{n} \left(\frac{y_{ki}}{\sqrt{\sum_{k=1}^{n} y_{ki}^{2}}} - \frac{y_{kj}}{\sqrt{\sum_{k=1}^{n} y_{kj}^{2}}} \right)^{2}}$$

The ChD is the maximum difference between variables. It gives even more weight to a outlying variable than the ED. The ChD is defined as

$$ChD = MAX_k |y_{ki} - y_{ki}|$$

Summarizing and optimizing the prediction

In our model, the prediction phase consists of summarizing the most similar cases in a prediction and creating the output. The prediction involves calculating some kind of weighted mean values for all endpoints and all effect classes for the most similar cases. For this purpose, the response variables of the *n* nearest cases are weighted in such a way that the influence of the cases declines with their dissimilarity from the question case. This prediction method is called the inverse distance method

$$prediction = \frac{\sum_{i=1}^{n} (y_{ki} \cdot D_i^p)}{\sum_{i=1}^{n} D_i^p}$$

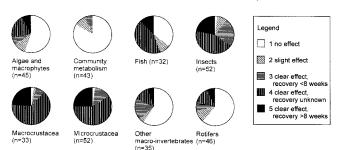


Fig. 2. Example of output from the model for predicting the ecological risks of pesticides (PERPEST) summarizing the prediction.

in which D is the chosen distance measure and p is the distance weighting power (negative). This prediction is done for each effect class of each grouped endpoint.

A bootstrapping procedure calculates the confidence intervals for the different effect classes and endpoints [17]. In this resampling technique, many (default 500) random data sets are generated by selecting cases at random, with replacement. We opt for a conservative approach by selecting a smaller number of cases than in the original database (default 75%). Each data set is used to produce a prediction. The generated distribution of predictions serves as an estimate of the uncertainty. The 2.5 and 97.5% percentiles from this bootstrap distribution serve as the 95% confidence interval.

Summarizing prediction. The prediction is summarized in a pie chart for each group of endpoints (see Fig. 2 for an example). These pie charts indicate the probability that the indicated changes in the grouped endpoints will fit into a particular effect class. This figure shows, for instance, that a 1% chance exists that an application of $10~\mu g/L$ chlorpyrifos will have no effect on the invertebrate group of Insecta (effect class 1). The figure also indicates that a large probability (92%) exists that clear effects will occur (effect classes 3, 4, and 5). For each class, the bootstrapped 95% confidence limits are presented in a table.

Goodness of fit. The performance of the prediction method is evaluated by using leave-one-out cross-validation [18], a technique in which one case is removed from the database, after which the effect on each endpoint group is predicted by using all other cases. The prediction is compared with the removed case. This procedure is repeated for all cases and in our case the log (likelihood) is determined as a goodness-of-fit measure because our effect classes are binary data.

Optimizing the prediction. The CBR methodology implies many subjective choices of the ranges and weights of parameters. We used the controlled random search procedure [19,20] to optimize these choices. The basis of this method is that the weights of each variable are tried at random within certain limits. The log (likelihood) of each trial is then determined by using the above cross-validation procedure. The controlled random search algorithm is used to find the optimum ranges and weights, that is, the values with the maximum goodness of fit.

Learning

As time passes, more experiments will be conducted and described in the open literature. Of all publications reviewed for our case base, one-third were published between 1995 and 1998, which means that PERPEST has gained one-third of its knowledge during this period. The results of newly published experiments can easily be added to PERPEST to improve fu-

Table 2. Properties of the herbicide methabenzthiazuron relevant to the PERPEST model for predicting the ecological risks of pesticides

Variable		Value
CAS	Chemical abstract service (CAS) registration number	18691-97-9
DT50	Median dissipation time in water phase of	
	water-sediment experiment	_
FullName	Full name of active ingredient	Methabenzthiazuron
Henry	Henry coefficient	_
K_{OM}	Organic matter partitioning coefficient	_
L(E)C50	Median lethal concentration (LC50) or median effect concentration (EC50) of most	
	susceptible standard test species	42.4
Mode of action	For example, photosynthesis inhibitor	Photosynthesis inhibitor
Molecule group	For example, triazin(on)e	Urea
Type_sub	Insecticide, herbicide, or fungicide	Herbicide

ture predictions. After new cases have been added, the weights and ranges of parameters can be optimized by using the new case base.

EXAMPLE OF THE APPLICATION OF THE MODEL

As an example of the application of the model, we predicted the ecological effects of methabenzthiazuron, a substance that has not yet been included in the database. Wellmann et al. [21] studied the effects of a single application of this herbicide on community metabolism (dissolved oxygen and pH) and species belonging to the phytoplankton, macrophyte, and zooplankton communities. The evaluated concentrations ranged from 10 to 3,371 μ g/L. The physicochemical and biological parameters were sampled from days 0 through 133 after application.

The first step in the prediction procedure is to enter the relevant data of the new substance in the database (Table 2). The second step is to optimize the weights and other properties by using controlled random search and cross-validation. A problem of optimizing was that effects of several parameters were correlated; the same goodness of fit could be obtained with several different parameter settings. Therefore, we did not optimize all parameters, but set several parameters to fixed values. Also, at least one weight of the conditional variable should be fixed, to avoid many possible combinations of weights yielding the same model. The absolute values of the weights are irrelevant; it is the relative values that matter. After optimization, the log (likelihood) was improved from -606 for the default settings, to -477 for the optimized model (Table 3).

In addition to the optimization, we conducted a simple sensitivity analysis: 2,000 random parameter sets were created,

varying the parameters within the same ranges as those used for the optimization. Subsequently, the log (likelihood) of each parameter set was calculated by using cross-validation. The sensitivity of the goodness of fit to parameter changes was calculated as the correlation between the values of each parameter and the log (likelihood) of the resulting model. The range of the TU, the maximum distance (for scaling), and the distance power were the most sensitive parameters; the weights of the variables were less critical.

We used the resulting optimized model to predict the effect of methabenzthiazuron on community metabolism, macrophytes, phytoplankton, and zooplankton (Fig. 3). The PER-PEST model predicted a dose-response relationship for the ecological endpoints. However, the exact concentration at which the effect starts was more difficult to predict. The noobserved-effect concentrations (NOECs) found in the semifield experiment for community metabolism and primary producers correspond with the predicted probability of clear effects, that is, approximately 50% (Fig. 3A to C). Above these NOECs, clear effects were found and predicted by PERPEST with a probability of more than 60%. Clear effects on zooplankton were recorded in the microcosm study at a concentration corresponding with the predicted probability of clear effects, that is, approximately 30% (Fig. 3D). The predicted and observed effects are in reasonable agreement.

DISCUSSION

In PERPEST, the concentrations evaluated in the microcosm and mesocosm experiments are standardized on the toxicity of the pesticide. This is done to make the exposure con-

Table 3. Improvement in fit (log [likelihood]) caused by optimization. The correlation between the value of the parameter and the log (likelihood) is shown in the last column. These coefficients have been determined with the goodness of fit of 2,000 random parameter sets. High absolute values indicate a high sensitivity of the model to this parameter

	Default settings	Optimized	Correlation
Log (likelihood)	-606	-477	
Number of cases for averaging	50	37	-0.05
Distance power	-2	-0.52	0.23
Minimum distance (fixed in optimizing)	1	1	-0.11
Maximum distance (fixed in optimizing)	10	10	0.26
Weight of toxic unit	1	6.3	-0.03
Weight of mode of action (fixed in optimizing)	1	1	0.04
Weight of molecule group (fixed in optimizing)	1	0	0.00
Weight of type of experiment (fixed in optimizing)) 1	0	-0.01
Weight of exposure (fixed in optimizing)	1	0	-0.03
Relative range of toxic unit	10	15.3	0.54

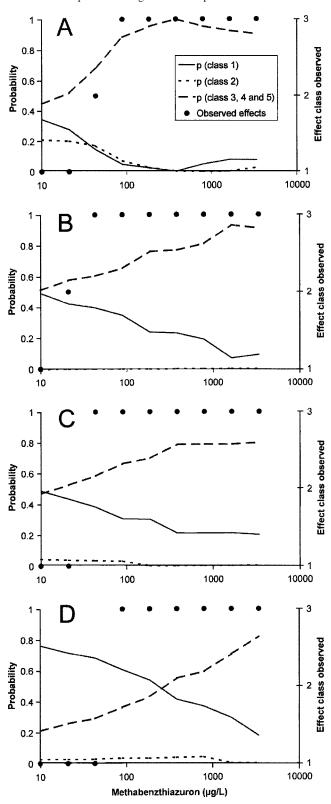


Fig. 3. Observed and predicted effects of methabenzthiazuron on community metabolism (\mathbf{A}), macrophytes (\mathbf{B}), phytoplankton (\mathbf{C}), and zooplankton (\mathbf{D}). Classes 3, 4, and 5 were combined for clarity.

centrations comparable between different pesticides. The standardization is based on the geometric mean EC50 of the most susceptible standard test species. The argument can be made that the EC50 of the susceptible group would reflect the toxicity of the pesticide better, because more information on the

community is used to derive this concentration. For this EC50, the median hazard concentration (HC50) and HC5 derived by using the species sensitivity distribution concept can be used. However, these effect concentrations are not derived in a uniform way and also are not readily available [22].

Pesticides have different toxicological profiles, even if, for instance, the molecule group to which they belong is similar. For instance, the toxicity of an insecticide to Daphnia and fish may be very similar or may differ greatly. This difference in toxicity becomes important, for instance, in predicting the effects on fish when using concentrations standardized on the toxicity for Daphnia. In such cases, it may be useful to add more toxicological information than just the geometric mean EC50 of the most sensitive standard test species. This toxicological information can be used to look for analogies in toxicological profiles of the different pesticides evaluated. This information is also needed when the effects of fungicides are added to the database. It is often not clear which (group of) endpoints are sensitive to fungicides [23], so one should preferably add as much available toxicity information as possible to the routine that searches for analogous cases. Also recommended is inclusion of field-derived DT50 values instead of laboratory-derived fate characteristics in the weighting of the different cases. However, such values are not widely available, and also depend on the ecosystem structure. Therefore, these field dissipations should be determined for the same experiments as those evaluated in Brock et al. [2,3].

In addition to predicting the effects of a single concentration, PERPEST is also able to construct concentration-effect curves for a range of concentrations of a particular pesticide. These curves describe the relationship between the concentration of a chemical and the probability that a particular effect (e.g., clear effects on insects) will occur. This concentrationeffect relationship for field effects allows better comparisons between laboratory- and field-derived effect curves than the use of point estimates such as NOEC_{ecosystems} [24,25]. This fullcurve comparison of laboratory and field effects enhances the verification of ecological risk assessment concepts based on laboratory toxicity data (e.g., species sensitivity distribution concept). Another advantage of these full-curve descriptions of field effects is that trigger values can be derived, based on a particular probability (e.g., 5%) that a particular effect (e.g., clear effects on a susceptible group) will occur.

This paper has presented a model that predicts the effects of pesticides based on historical, empirical data. However, it may be questioned whether enough empirical data are available to allow such predictions to be made. The current shortage of empirical data is reflected in the 95% confidence intervals of the predictions, which are usually quite large when probabilities around 50% are predicted. On the other hand, models of biological systems often are incomplete, either because a complete state description for such systems cannot be provided or because the numbers and types of interactions between system elements are poorly understood [26]. Therefore, Scheffer [27] proposed an integration of experimental data and models by starting from the assumption that the effect to be predicted will be analogous to that of the same measure elsewhere and by using quantitative models only to correct for expected differences. Branting et al. [26] called this integration of CBR and model-based reasoning model-based adaptation, and described an example involving a system for rangeland grasshopper management. In the light of the tiered approach that has been adopted in risk assessment and the availability of models, this integration looks promising for the field of ecological risk assessment of pesticides for their registration on the European market [1].

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REFERENCES

- 1. Campbell PJ, Arnold DJS, Brock TCM, Grandy NJ, Heger W, Heimbach F, Maund SJ, Streloke M. 1999. *Guidance Document on Higher Tier Aquatic Risk Assessment for Pesticides (HARAP)*. SETAC-Europe, Brussels, Belgium.
- Brock TCM, Lahr J, Van den Brink PJ. 2000. Ecological risks of pesticides in freshwater ecosystems. Part 1: Herbicides. Final Report 088. Alterra Green World Research, Wageningen, The Netherlands.
- Brock TCM, Van Wijngaarden RPA, Van Geest GJ. 2000. Ecological risks of pesticides in freshwater ecosystems. Part 2: Insecticides. Final Report 089. Alterra Green World Research, Wageningen, The Netherlands.
- Koelmans AA, Van der Heijde A, Knijff L, Aalderink RH. 2001. Modelling feedbacks between eutrophication and organic contaminant fate and effects in aquatic ecosystems. A review. Water Res 35:3517–3536.
- Traas TP, Janse JH, Aldenberg T, Brock TCM. 1998. A food web model for fate, direct and indirect effects of Dursban 4E (a.i. chlorpyrifos) in freshwater microcosms. Aquat Ecol 32:179–190.
- Anderson JR. 1983. The Architecture of Cognition. Harvard University Press, Cambridge, UK.
- 7. Kolodner JL. 1993. *Case-Based Reasoning*. Morgan Kaufmann, San Mateo, CA, USA.
- 8. Leake BD. 1996. Case-Based Reasoning. Experiences, Lessons and Future Directions. AAAI, Menlo Park, CA, USA.
- Van Nes EH, Scheffer M. 1993. Best Analogous Situations Information Systems. User's Guide for BASIS, Ver 1.0. Final Report 93.044. Institute for Inland Water Management and Waste Water Treatment (RIZA), Lelystad, The Netherlands.
- Aamodt A, Plaza E. 1994. Case-based reasoning: Foundational issues, methodological variations, and system approaches. AI Commun 7:39-59.
- Schank R. 1982. Dynamic Memory; A Theory of Reminding and Learning in Computers and People. Cambridge University Press, Cambridge, UK.
- Kolodner JL. 1983. Maintaining organization in a dynamic longterm memory. Cognit Sci 7:243–280.
- Watson I, Marir F. 1994. Case-based reasoning: A review. Knowledge Eng Rev 9:355–381.
- Frize M, Walker R. 2000. Clinical decision-support systems for intensive care units using case-based reasoning. *Med Eng Phys* 22:671–677.
- Montani S, Bellazzi R, Portinale L, d'Annunzio G, Fiocchi S, Stefanelli M. 2000. Diabetic patients management exploiting case-based reasoning techniques. *Comput Methods Programs Biomed* 62:205–218.
- Jongman RHG, Ter Braak CJF, Van Tongeren OFR. 1995. Data Analysis in Community and Landscape Ecology. Cambridge University Press, Cambridge, UK.

- 17. Manly BFJ. 1997. Randomization, Bootstrap and Monte Carlo Methods in Biology. Chapman & Hall, London, UK.
- Stone M. 1974. Cross-validatory choice and assessment of statistical predictions. J R Stat Soc B 36:111–147.
- Price WL. 1977. A controlled random procedure for global optimisation. Computer J 20:367–370.
- Klepper O, Hendrix EMT. 1994. A comparison of algorithms for global characterization of confidence regions for nonlinear models. *Environ Toxicol Chem* 13:1887–1899.
- Wellmann P, Ratte HT, Heimbach F. 1998. Primary and secondary effects of methabenzthiazuron on plankton communities in aquatic outdoor microcosms. Aquat Ecol 32:125–134.
- Posthuma L, Traas TP, Suter GW. 2002. The Use of Species Sensitivity Distributions in Ecotoxicology. Lewis, Boca Raton, FL, USA
- Cuppen JGM, Van den Brink PJ, Uil KF, Camps E, Brock TCM. 2000. Impact of the fungicide carbendazim in freshwater microcosms. I Water quality, breakdown of particulate organic matter and responses of macro-invertebrates. *Aquat Toxicol* 48:233–250.
- Versteeg DJ, Belanger SE, Carr GJ. 1999. Understanding singlespecies and model ecosystem sensitivity: Data based comparison. *Environ Toxicol Chem* 18:1329–1346.
- 25. Van den Brink PJ, Posthuma L, Brock TCM. 2002. The value of the species sensitivity distribution concept for predicting field effects: (Non)confirmation of the concept using semi-field experiments. In Posthuma L, Traas TP, Suter GW, eds, *The Use of Species Sensitivity Distributions in Ecotoxicology*. Lewis, Boca Raton, FL, USA, pp 155–193.
- Branting LK, Hastings JD, Lockwood JA. 1997. Integrating cases and models for predictions in biological systems. AI Appl 11:29– 48.
- Scheffer M. 1991. On the predictability of aquatic vegetation in shallow lakes. In Ecosystem research in freshwater environment recovery. *Mem Ist Ital Idrobiol* 48:207–217.
- DeNoyelles F, Kettle WD, Sinn DE. 1982. The responses of plankton communities in experimental ponds to atrazine, the most heavily used pesticide in the United States. *Ecology* 63:1285– 1293
- DeNoyelles F, Kettle WD, Fromm CH, Moffett MF, Dewey SL. 1989. Use of experimental ponds to assess the effects of a pesticide on the aquatic environment. *Entomol Soc Am Misc Publ* 75:41–56.
- DeNoyelles F, Dewey SL, Huggins DG, Kettle WD. 1994. Aquatic mesocosms in ecological effects testing: Detecting direct and indirect effects of pesticides. In Graney RL, Kennedy JH, Rodgers JH, eds, Aquatic Mesocosm Studies in Ecological Risk Assessment. Lewis, Boca Raton, FL, USA, pp 577–603.
- 31. Brock TCM, Crum SJH, Van Wijngaarden RPA, Budde BJ, Tijink J, Zupelli A, Leeuwangh P. 1992. Fate and effects of the insecticide Dursban® 4E in indoor *Elodea*-dominated and macrophyte-free freshwater model ecosystems: I. Fate and primary effects of the active ingredient chlorpyrifos. *Arch Environ Contam Toxicol* 23:69–84.
- 32. Brock TCM, Van den Bogaert M, Bos AR, Van Breukelen SWF, Reiche R, Terwoert J, Suykerbuyk REM, Roijackers RMM. 1992b. Fate and effects of the insecticide Dursban® 4E in indoor *Elodea*-dominated and macrophyte-free freshwater model ecosystems: II. Secondary effects on community structure. *Arch Environ Contam Toxicol* 23:391–409.
- 33. Brock TCM, Vet JJRM, Kerkhofs MJJ, Lijzen J, Van Zuilekom WJ, Gijlstra R. 1993. Fate and effects of the insecticide Dursban® 4E in indoor *Elodea*-dominated and macrophyte-free freshwater model ecosystems: III. Aspects of ecosystem functioning. *Arch Environ Contam Toxicol* 25:160–169.